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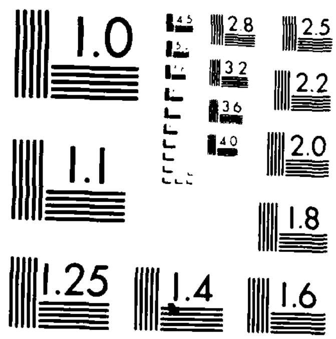

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This paper introduces two design criteria to improve the power of the multivariate lack of fit test for a linear multiresponse model. An algorithm is presented for the generation of optimal designs on the basis of these criteria.

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CONSTRUCTION OF OPTIMAL DESIGNS TO INCREASE THE POWER OF THE MULTIRESPONSE LACK OF FIT TEST

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Abstract: Two design criteria are introduced to improve the power of the multivariate lack of fit test for a linear multiresponse model. These criteria are extensions of the Λ_1 and Λ_2-optimality criteria discussed by Jones and Mitchell (1978) for the single-response case. A procedure is presented for the generation of an optimal design based on the Λ_2-criterion.

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Key words and phrases: Multiresponse design; Λ_1-optimality; Λ_2-optimality; Multivariate lack of fit test.

1. Introduction

Detection of model inadequacy is an important consideration in the modeling of a multiresponse function. Khuri (1985) developed a multivariate test for lack of fit for a linear multiresponse model. The test provides a comprehensive assessment of the adequacy of all the single-response functions associated with the multiresponse model. He also gave a procedure for determining which responses are responsible for lack of fit when the lack of fit test is significant.

In Section 2 we introduce some notation and briefly discuss Khuri's (1985) lack of fit test. In Section 3 we develop two design criteria, Λ_1 and Λ_2-optimality, to increase the power of this test. In Section 4 an iterative procedure developed by Silvey (1980) is used to obtain Λ_2-optimal designs. Numerical examples are presented in Section 5.

2. The Multiresponse Lack of Fit Test

2.1 Notation

Let N be the total number of experimental runs and r be the number of responses. We assume that each response depends on all or some of k controllable variables denoted by $x_1, x_2, \ldots, x_k$. The fitted ith response model is represented as

$$E_a(\underset{\sim}{Y}_i) = \underset{\sim}{X}_i \underset{\sim}{\beta}_i, \quad i = 1,2,\ldots,r, \tag{1}$$

where $\underset{\sim}{Y}_i$ is an N×1 vector of observations on the ith response, $E_a(\underset{\sim}{Y}_i)$ denotes the expected value of $\underset{\sim}{Y}_i$ under the fitted model, $\underset{\sim}{X}_i$ is an $N \times p_i$ matrix of rank p_i of known functions of the settings of the controllable variables, and $\underset{\sim}{\beta}_i$ is a $p_i \times 1$ vector of unknown parameters (i=1,2,...,r).

We suppose that the model for the true ith response mean (i=1,2,...,r) is of the form

$$E_t(\underset{\sim}{Y}_i) = \underset{\sim}{X}_i \underset{\sim}{\beta}_i + \underset{\sim}{Z}_i \underset{\sim}{\gamma}_i, \quad i=1,2,\ldots,r, \tag{2}$$

where $E_t(\underset{\sim}{Y}_i)$ denotes the expected value of $\underset{\sim}{Y}_i$ under the true model, $\underset{\sim}{Z}_i$ is an $N \times q_i$ matrix of known functions of the settings of the controllable variables,

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and $\underset{\sim}{\gamma}_i$ is a vector of unknown parameters. If the fitted model (1) is correct, then $\underset{\sim}{\gamma}_i$ will be equal to the zero vector.

The models given in (1) and (2) can be expressed as

$$E_a(\underset{\sim}{Y}) = \underset{\sim}{X}\underset{\sim}{B} \tag{3}$$

$$E_t(\underset{\sim}{Y}) = \underset{\sim}{X}\underset{\sim}{B} + \underset{\sim}{Z}\underset{\sim}{\Gamma}, \tag{4}$$

where $\underset{\sim}{Y} = [\underset{\sim}{Y}_1 : \underset{\sim}{Y}_2 : \ldots : \underset{\sim}{Y}_r]$, $\underset{\sim}{X} = [\underset{\sim}{X}_1 : \underset{\sim}{X}_2 : \ldots : \underset{\sim}{X}_r]$, $\underset{\sim}{Z} = [\underset{\sim}{Z}_1 : \underset{\sim}{Z}_2 : \ldots : \underset{\sim}{Z}_r]$, $\underset{\sim}{B} = \mathrm{diag}(\underset{\sim}{\beta}_1, \underset{\sim}{\beta}_2, \ldots, \underset{\sim}{\beta}_r)$, and $\underset{\sim}{\Gamma} = \mathrm{diag}(\underset{\sim}{\gamma}_1, \underset{\sim}{\gamma}_2, \ldots, \underset{\sim}{\gamma}_r)$. The matrices $\underset{\sim}{Y}$, $\underset{\sim}{X}$, $\underset{\sim}{Z}$, $\underset{\sim}{B}$, and $\underset{\sim}{\Gamma}$ are of orders $N \times r$, $N \times p$, $N \times q$, $p \times r$, and $q \times r$, respectively, where $p = \sum_{i=1}^{r} p_i$, $q = \sum_{i=1}^{r} q_i$, and $\underset{\sim}{X}$ is of rank ρ ($\leq p$). The rows of $\underset{\sim}{Y}$ are independent observations from multivariate normal populations with a common nonsingular variance-covariance matrix $\underset{\sim}{\Sigma}$ of order $r \times r$. Under the true model, $\underset{\sim}{Y}$ has a mean given by (4) and a variance-covariance matrix $\underset{\sim}{I}_N \otimes \underset{\sim}{\Sigma}$.

For the development of the lack of fit test we assume that replicated observations are available on all r responses at some points in the experimental region. Without loss of generality, it will be assumed that such replicated observations are obtained at each of the first n design points, where $1 \leq n < N$. The number of repeated observations at the ith design point is denoted by ν_i ($\nu_i \geq 2$, $i = 1,2,\ldots,n$) and the total number of repeated observations is $\nu = \sum_{i=1}^{n} \nu_i$.

2.2 Khuri's (1985) Lack of Fit Test

Let $\underset{\sim}{X}_0$ denote the matrix which consists of the columns of $\underset{\sim}{X}$ that correspond to all distinct terms in the r fitted models given in (1). The columns of $\underset{\sim}{X}_0$ span the column space of $\underset{\sim}{X}$. We, therefore, consider that $\underset{\sim}{X}_0$ is of full column rank equal to ρ, the rank of $\underset{\sim}{X}$. Khuri (1985) developed a multivariate lack of fit test for the multiresponse model (3) using

$e_{max}(\underset{\sim}{G}_1\underset{\sim}{G}_2^{-1})$, the maximum eigenvalue of the matrix $\underset{\sim}{G}_1\underset{\sim}{G}_2^{-1}$, as a test statistic, where

$$\begin{aligned} \underset{\sim}{G}_1 &= \underset{\sim}{Y}'[\underset{\sim}{I}_N - \underset{\sim}{X}_0(\underset{\sim}{X}_0'\underset{\sim}{X}_0)^{-1}\underset{\sim}{X}_0' - \underset{\sim}{K}]\underset{\sim}{Y} \\ \underset{\sim}{G}_2 &= \underset{\sim}{Y}'\underset{\sim}{K}\underset{\sim}{Y} . \end{aligned} \tag{5}$$

In the above equations, $\underset{\sim}{K} = \text{diag}(\underset{\sim}{K}_1, \underset{\sim}{K}_2, \ldots, \underset{\sim}{K}_n, \underset{\sim}{0})$ is of order $N\times N$ with $\underset{\sim}{0}$ being a zero matrix of order $(N-\nu)\times(N-\nu)$ and $\underset{\sim}{K}_i = \underset{\sim}{I}_{\nu_i} - (1/\nu_i)\underset{\sim}{J}_{\nu_i}$, where $\underset{\sim}{I}_{\nu_i}$ is the identity matrix of order $\nu_i\times\nu_i$ and $\underset{\sim}{J}_{\nu_i}$ is the matrix of ones of order $\nu_i\times\nu_i$ $(i=1,2,\ldots,n)$. Three other test statistics can also be employed to test lack of fit; they are: (1) Wilks's likelihood ratio, $|\underset{\sim}{G}_2|/|\underset{\sim}{G}_1 + \underset{\sim}{G}_2|$; (2) Pillai's trace, tr $[\underset{\sim}{G}_1(\underset{\sim}{G}_1 + \underset{\sim}{G}_2)^{-1}]$; and (3) Hotelling-Lawley's trace, tr $(\underset{\sim}{G}_1\underset{\sim}{G}_2^{-1})$, where $|\;|$ and tr denote the determinant and the trace of a matrix, respectively.

3. Development of Design Criteria

It is known that $\underset{\sim}{G}_2$ has the central Wishart distribution with $\nu_{PE} = \sum_{i=1}^{n}(\nu_i - 1)$ degrees of freedom; $\underset{\sim}{G}_1$ is independent of $\underset{\sim}{G}_2$ and has the noncentral Wishart distribution with $\nu_{LF} = (N-\rho-\nu_{PE})$ degrees of freedom and a noncentrality parameter matrix given by

$$\underset{\sim}{\Omega} = \underset{\sim}{\Sigma}^{-1}\underset{\sim}{\Gamma}'\underset{\sim}{Z}'[\underset{\sim}{I}_N - \underset{\sim}{X}_0(\underset{\sim}{X}_0'\underset{\sim}{X}_0)^{-1}\underset{\sim}{X}_0']\underset{\sim}{Z}\underset{\sim}{\Gamma}. \tag{6}$$

The power of the lack of fit test, based upon any of the four multivariate test statistics mentioned earlier, is a monotone increasing function of the eigenvalues of $\underset{\sim}{\Omega}$ (see Roy et al. 1971, p. 68). Therefore, the power of this test can be increased by increasing the trace of $\underset{\sim}{\Omega}$. However, the choice of the design which maximizes the trace of $\underset{\sim}{\Omega}$ depends on the matrices $\underset{\sim}{\Sigma}$ and $\underset{\sim}{\Gamma}$ which are unknown. Thus, we are faced with the problem of finding an expression independent of Σ and Γ which, when maximized, results in an increase in the trace of Ω. This expression is found as follows: It is easy to show that

$$\mathrm{tr}(\Omega) > e_{min}(\Sigma^{-1})\ \mathrm{tr}[\Gamma'Z'\{I_N - X_0(X_0'X_0)^{-1}X_0'\}Z\Gamma], \tag{7}$$

where e_{min} denotes the smallest eigenvalue of the matrix inside parentheses. Inequality (7) can be rewritten as (see the Appendix)

$$\mathrm{tr}(\Omega) > e_{min}(\Sigma^{-1})\gamma'L(I_r \otimes A)L'\gamma, \tag{8}$$

where

$$\gamma' = [\gamma_1' : \gamma_2' : \ldots : \gamma_r'], \tag{9}$$

$$A = Z_0'\{I_N - X_0(X_0'X_0)^{-1}X_0'\}Z_0, \tag{10}$$

$$L = \mathrm{diag}(H_1', H_2', \ldots, H_r'). \tag{11}$$

In (10), Z_0 is a matrix of order $N \times \rho_1 (\rho_1 < q)$ whose columns form a basis for the column space of $Z = [Z_1 : Z_2 : \ldots : Z_r]$. Thus,

$$Z_i = Z_0 H_i\ , \quad i = 1, 2, \ldots, r, \tag{12}$$

where H_i is matrix of order $\rho_1 \times q_i$.

Since $e_{min}(\Sigma^{-1})$ is a constant, the maximization of the quantity

$$\Lambda = \gamma'L\ (I_r \otimes A)\ L'\gamma \tag{13}$$

will result in an increase in the trace of Ω. Still, however, the choice of design to maximize Λ depends on γ which is unknown. In order to overcome this problem we apply the maximin method proposed by Atkinson and Fedorov (1975) and used by Jones and Mitchell (1978) in the single-response case. The maximin method consists of choosing a design which maximizes Λ_1, the minimum of Λ with respect to γ over a specified region π in the γ-space. The specification of the region π depends on a quantity τ considered as a measure of the inadequacy of the fitted model and is defined as follows: Suppose the uth rows of $\underset{\sim}{X}_i$ and $\underset{\sim}{Z}_i$ ($i=1,2,\ldots,r$; $u=1,2,\ldots,N$) in (2) can be represented as $\underset{\sim}{f}_i'(\underset{\sim}{x}_u)$ and $\underset{\sim}{g}_i'(\underset{\sim}{x}_u)$, respectively, then the fitted and true response functions associated with (1) and (2) are $\underset{\sim}{f}_i'(\underset{\sim}{x})\underset{\sim}{\beta}_i$ and $\underset{\sim}{f}_i'(\underset{\sim}{x})\underset{\sim}{\beta}_i + \underset{\sim}{g}_i'(\underset{\sim}{x})\underset{\sim}{\gamma}_i$ ($i = 1,2,\ldots,r$), respectively. We express τ as $\tau = \underset{\sim}{\gamma}'\underset{\sim}{T}\underset{\sim}{\gamma}$, where

$$\underset{\sim}{T} = \mathrm{diag}\left(\underset{\sim}{T}_1, \underset{\sim}{T}_2, \ldots, \underset{\sim}{T}_r\right) \tag{14}$$

with $\underset{\sim}{T}_i = \underset{\sim}{\mu}_{22}^i - \underset{\sim}{\mu}_{21}^i(\underset{\sim}{\mu}_{11}^i)^{-1}\underset{\sim}{\mu}_{12}^i$ and the $\underset{\sim}{\mu}_{k\ell}^i$ ($k, \ell = 1,2$) are the region moment matrices defined by $\underset{\sim}{\mu}_{11}^i = S\int_X \underset{\sim}{f}_i(\underset{\sim}{x})\underset{\sim}{f}_i'(\underset{\sim}{x})d\underset{\sim}{x}$, $\underset{\sim}{\mu}_{12}^i = S\int_X \underset{\sim}{f}_i(\underset{\sim}{x})\underset{\sim}{g}_i'(\underset{\sim}{x})d\underset{\sim}{x}$, $\underset{\sim}{\mu}_{21}^i = S\int_X \underset{\sim}{g}_i(\underset{\sim}{x})\underset{\sim}{f}_i'(\underset{\sim}{x})d\underset{\sim}{x}$, and $\underset{\sim}{\mu}_{22}^i = S\int_X \underset{\sim}{g}_i(\underset{\sim}{x})\underset{\sim}{g}_i'(\underset{\sim}{x})d\underset{\sim}{x}$, where $S^{-1} = \int_X d\underset{\sim}{x}$ and X denotes the experimental region. This is a multiresponse extension of the expression for τ given by Jones and Mitchell (1978). It is a measure of the inadequacy of the fitted models given in (1) and is positive whenever the fitted model is inadequate, otherwise, it is equal to zero.

3.1 Λ_1-Optimality

If the fitted model is inadequate, then $\tau > \delta$ for some constant $\delta > 0$. We define $\pi = \{\underset{\sim}{\gamma} : \underset{\sim}{\gamma}'\underset{\sim}{T}\underset{\sim}{\gamma} > \delta\}$. The first design criterion is to maximize Λ_1 where

$$\Lambda_1 = \inf_{\underset{\sim}{\gamma}\in\pi} \left\{\underset{\sim}{\gamma}'\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{A})\ \underset{\sim}{L}'\underset{\sim}{\gamma}\right\}. \tag{15}$$

This is a multiresponse extension of the Λ_1-optimality criterion proposed by Jones and Mitchell (1978). As in Jones and Mitchell (1978), Λ_1 can be expressed as

$$\Lambda_1 = \delta\ e_{\min}\{\underset{\sim}{T}^{-1}\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{A})\underset{\sim}{L}'\}. \tag{16}$$

A design which maximizes $e_{\min}\{\underset{\sim}{T}^{-1}\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{A})\underset{\sim}{L}'\}$ is called a Λ_1-optimal design. Note that there are situations in which $e_{\min}\{\underset{\sim}{T}^{-1}\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{A})\underset{\sim}{L}'\}$ is equal to zero for any choice of design. This occurs, for example, when $r(N-\rho) < q$, where ρ is the number of columns of $\underset{\sim}{X}_0$ and $q = \sum_{i=1}^{r} q_i$ is the number of columns in $\underset{\sim}{Z}$ in (4), or the number of rows of the matrix $\underset{\sim}{L}$ in (11). In this case the rank of the $q\times q$ matrix $\underset{\sim}{T}^{-1}\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{A})\underset{\sim}{L}'$ is less than or equal to $r(N-\rho)$ which is less than q. This matrix is, therefore, singular. Thus, Λ_1-optimal designs can only be obtained under certain conditions. This leads us to propose a second design criterion which can be applied in more general situations.

3.2 <u>Λ_2-Optimality</u>

Our second design criterion is to maximize Λ_2, the average of Λ (instead of the minimum of Λ) over the contour $\tau = \delta$, i.e., we propose to select a design which maximizes

$$\Lambda_2 = \int_{\pi_0} \underset{\sim}{\gamma}'\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{A})\underset{\sim}{L}'\underset{\sim}{\gamma}\, dG \Big/ \int_{\pi_0} dG, \tag{17}$$

where dG is the differential of the area on the surface of the ellipsoid $\pi_0 = \{\underset{\sim}{\gamma}:\underset{\sim}{\gamma}'\underset{\sim}{T}\underset{\sim}{\gamma} = \delta\}$. Using an identity stated in Jones and Mitchell (1978, p. 544) we have that

$$\Lambda_2 = q^{-1}\delta\,\Lambda_2', \text{ where } \Lambda_2' = \mathrm{tr}\{\underset{\sim}{T}^{-1}\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{A})\underset{\sim}{L}'\}. \tag{18}$$

A design which maximizes Λ_2, or Λ_2', is called a Λ_2-optimal (Λ_2'-optimal) design. Since q and δ are constants it is clear that Λ_2-optimal designs and Λ_2'-optimal designs are equivalent. We note that the Λ_2-optimality criterion amounts to maximizing the sum of the eigenvalues of $\underset{\sim}{T}^{-1}\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{A})\underset{\sim}{L}'$; hence, it can be applied even when this matrix has a zero eigenvalue.

If the number of design points, N, is fixed beforehand, a Λ_2-optimal design can be obtained by maximizing Λ_2' with respect to the Nk design setting (coordinates of the N design points). However, this may lead to computational difficulties especially for large values of N or k. Therefore, an iterative procedure by which design points can be chosen one at a time would be quite desirable. In the next section we develop such a procedure by using single-response optimal design theory.

4. The Generation of Λ_2'-Optimal Designs

4.1 Design Theory

Consider the single-response model

$$E(y_{\underset{\sim}{x}}) = \underset{\sim}{h}'(\underset{\sim}{x})\underset{\sim}{\theta}, \tag{19}$$

where $y_{\underset{\sim}{x}}$ denotes the response value at a point $\underset{\sim}{x} = (x_1, x_2, \ldots, x_k)'$, the elements of the $m\times 1$ vector $\underset{\sim}{h}'(\underset{\sim}{x})$ are functions of $x_1, x_2, \ldots, x_k$ defined over some experimental region χ, a compact subset of the k-dimensional Euclidean space, and $\underset{\sim}{\theta}$ is a vector of unknown parameters. We assume that $\mathrm{Var}(y_{\underset{\sim}{x}}) = \sigma^2$, $\mathrm{Cov}(y_{\underset{\sim}{x}_1}, y_{\underset{\sim}{x}_2}) = 0$ for $\underset{\sim}{x}$, $\underset{\sim}{x}_1$, $\underset{\sim}{x}_2$ in $\chi(\underset{\sim}{x}_1 \neq \underset{\sim}{x}_2)$. Let H be the set of all design measures defined on χ. Then the information matrix $\underset{\sim}{M}(\zeta)$, $\zeta\varepsilon H$, is defined as

$$\underset{\sim}{M}(\zeta) = \int_{\chi} \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})\zeta(d\underset{\sim}{x}). \tag{20}$$

The family of matrices, $\mathcal{M} = \{\underset{\sim}{M}(\zeta):\zeta\varepsilon H\}$, is convex (Silvey 1980, p. 16). By Carathéodory's Theorem, for any design measure ζ, the matrix $\underset{\sim}{M}(\zeta)$ can be represented in the form

$$\underset{\sim}{M}(\zeta) = \sum_{u=1}^{s} \lambda_u \underset{\sim}{h}(\underset{\sim}{x}_u)\underset{\sim}{h}'(\underset{\sim}{x}_u), \tag{21}$$

where $\underset{\sim}{x}_u \varepsilon \chi$ $(u = 1,2,\ldots,s)$, $s \leq m' = [m(m+1)/2] + 1$, and $0 \leq \lambda_u \leq 1$ with $\sum_{u=1}^{s} \lambda_u = 1$ (see Silvey 1980, pp. 15-16). Thus, for a given $\underset{\sim}{M}(\zeta)\varepsilon\mathcal{M}$ and $\underset{\sim}{\lambda}\varepsilon\,\mathcal{U} = \{\underset{\sim}{\lambda}:\underset{\sim}{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_{m'})'$ such that $0 \leq \lambda_u \leq 1$ and $\sum_{u=1}^{m'} \lambda_u = 1\}$,

there exists a point $\underset{\sim}{w}' = (\underset{\sim}{\lambda}', \underset{\sim}{x}_1', \underset{\sim}{x}_2', \ldots, \underset{\sim}{x}_{m'}')$ in $\mathcal{U} \times \chi^{m'}$ that is associated with $\underset{\sim}{M}(\zeta)$. Note that in $\underset{\sim}{\lambda}$, $\lambda_u = 0$ for $s < u \leq m'$. If ϕ is a real-valued function bounded from above on $\mathcal{M}$, then a design measure ζ^* is said to be

ϕ-optimal if

$$\phi[\underset{\sim}{M}(\zeta^*)] = \sup_{\zeta \varepsilon H} \phi[\underset{\sim}{M}(\zeta)]. \tag{22}$$

Silvey (1980, ch. 4) presented an iterative procedure to obtain ϕ-optimal designs. The basic idea used in this procedure (Silvey 1980, p. 29) is as follows: Suppose $D_N = \{\underset{\sim}{x}_1, \underset{\sim}{x}_2, \ldots, \underset{\sim}{x}_N\}$ represents an N-point discrete design and ζ_N is the design measure obtained by attaching the mass $\lambda_u = \frac{1}{N}$ $(u = 1,2,\ldots,N)$ to each design point in D_N. Start with an initial N_0-point design such that $\phi[\underset{\sim}{M}(\zeta_{N_0})] > -\infty$. Once D_N, hence ζ_N, $N > N_0$, has been determined, choose the design point $\underset{\sim}{x}_{N+1}$ such that

$$F_\phi\{\underset{\sim}{M}(\zeta_N),\ \underset{\sim}{h}(\underset{\sim}{x}_{N+1})\underset{\sim}{h}'(\underset{\sim}{x}_{N+1})\} = \sup_{\underset{\sim}{x} \varepsilon X} F_\phi\{\underset{\sim}{M}(\zeta_N), \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})\}, \tag{23}$$

where for $\underset{\sim}{M}_1, \underset{\sim}{M}_2$ in M, $F_\phi(\underset{\sim}{M}_1, \underset{\sim}{M}_2)$ is the Fréchet derivative of ϕ at $\underset{\sim}{M}_1$ in the direction of $\underset{\sim}{M}_2$ and is defined as

$$F_\phi(\underset{\sim}{M}_1, \underset{\sim}{M}_2) = \lim_{\varepsilon \to 0^+} (1/\varepsilon)[\phi\{(1-\varepsilon)\underset{\sim}{M}_1 + \varepsilon \underset{\sim}{M}_2\} - \phi(\underset{\sim}{M}_1)]. \tag{24}$$

The procedure is stopped when $\sup_{\underset{\sim}{x} \varepsilon X} F_\phi\{M(\zeta_{N'}),\ \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})\}$ is less than some small positive preset value for some $N' > N_0$. This stopping rule is based on the following lemma (Silvey 1980, p. 22):

<u>Lemma 1</u>. Let ϕ be concave on M and differentiable on $M' = \{\underset{\sim}{M}(\zeta): \underset{\sim}{M}(\zeta) \varepsilon M$ and $\phi[\underset{\sim}{M}(\zeta)] > -\infty\}$. Suppose a ϕ-optimal measure exists. Then ζ^* is ϕ-optimal if and only if

$$\sup_{\underset{\sim}{x} \varepsilon X} F_\phi\{\underset{\sim}{M}(\zeta^*),\ \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})\} = 0. \tag{25}$$

The sequence of design measures $\{\zeta_N\}$ defined in the iterative procedure obeys the recursive formula

$$\zeta_{N+1} = (1-\alpha_N)\zeta_N + \alpha_N \zeta(\underset{\sim}{x}_{N+1}), \tag{26}$$

where $\alpha_N = 1/(N+1)$ and $\zeta(\underset{\sim}{x}_{N+1})$ denotes the design measure which assigns 1 to the point $\underset{\sim}{x}_{N+1}$. Silvey (1980, pp. 35-36) shows that for such $\{\alpha_N\}$ the procedure converges.

Let us now consider the multiresponse model given in (3) and the Λ_2'-optimality criterion defined in Section 3.2. We shall apply Silvey's (1980) procedure to construct Λ_2'-optimal designs. For this purpose let us consider the matrices $\underset{\sim}{X}_0$ and $\underset{\sim}{Z}_0$, which are of orders $N\times\rho$ and $N\times\rho_1$ and appear in (5) and (12), respectively. We introduce a single-response model of the form given in (19) with $\underset{\sim}{h}'(\underset{\sim}{x}) = [\underset{\sim}{a}'(\underset{\sim}{x}) : \underset{\sim}{b}'(\underset{\sim}{x})]$, where $\underset{\sim}{a}'(\underset{\sim}{x})$ and $\underset{\sim}{b}'(\underset{\sim}{x})$ are vectors of dimensions ρ and ρ_1 that represent a row of $\underset{\sim}{X}_0$ and a corresponding row of $\underset{\sim}{Z}_0$, respectively, evaluated at a point $\underset{\sim}{x}$. The corresponding information matrix for a discrete N-point design measure ζ_N can be written as

$$\underset{\sim}{M}(\zeta_N) = \begin{bmatrix} \underset{\sim}{M}_{XX}(\zeta_N) & \underset{\sim}{M}_{XZ}(\zeta_N) \\ \underset{\sim}{M}_{ZX}(\zeta_N) & \underset{\sim}{M}_{ZZ}(\zeta_N) \end{bmatrix}, \tag{27}$$

where $\underset{\sim}{M}_{XX}(\zeta_N) = \underset{\sim}{X}_0' \underset{\sim}{X}_0/N$, $\underset{\sim}{M}_{XZ}(\zeta_N) = \underset{\sim}{X}_0' \underset{\sim}{Z}_0/N$, $\underset{\sim}{M}_{ZX}(\zeta_N) = \underset{\sim}{Z}_0' \underset{\sim}{X}_0/N$, and $\underset{\sim}{M}_{ZZ}(\zeta_N) = \underset{\sim}{Z}_0' \underset{\sim}{Z}_0/N$. The corresponding expression for Λ_2' in (18) can now be written as a function of $\underset{\sim}{M}(\zeta_N)$ of the form

$$\Lambda_2'[\underset{\sim}{M}(\zeta_N)] = \mathrm{tr}[\underset{\sim}{T}^{-1}\underset{\sim}{L}\{\underset{\sim}{I}_r \otimes \underset{\sim}{A}(\zeta_N)\}\underset{\sim}{L}'], \tag{28}$$

where $\underset{\sim}{A}(\zeta_N) = N[\underset{\sim}{M}_{ZZ}(\zeta_N) - \underset{\sim}{M}_{ZX}(\zeta_N)\underset{\sim}{M}_{XX}^{-1}(\zeta_N)\underset{\sim}{M}_{XZ}(\zeta_N)]$. In general, if ζ is any design measure defined on a compact subset, χ, of the k-dimensional Euclidean space, then an extension of the Λ_2' function in (28) when $\underset{\sim}{M}_{XX}(\zeta)$ is nonsingular is

$$\Lambda_2'[\underset{\sim}{M}(\zeta)] = \mathrm{tr}[\underset{\sim}{T}^{-1}\underset{\sim}{L}\{\underset{\sim}{I}_r \otimes \underset{\sim}{A}(\zeta)\}\underset{\sim}{L}'], \tag{29}$$

where $\underset{\sim}{A}(\zeta) = \underset{\sim}{M}_{ZZ}(\zeta) - \underset{\sim}{M}_{ZX}(\zeta)\underset{\sim}{M}_{XX}^{-1}(\zeta)\underset{\sim}{M}_{XZ}(\zeta)$ and $\underset{\sim}{M}_{XX}(\zeta)$, $\underset{\sim}{M}_{XZ}(\zeta)$, $\underset{\sim}{M}_{ZX}(\zeta)$, and $\underset{\sim}{M}_{ZZ}(\zeta)$ provide a partitioning of $\underset{\sim}{M}(\zeta)$ in (20) analogous to that of $\underset{\sim}{M}(\zeta_N)$ in

(27).

If H is the set of all design measures on χ and M is the set $\{\underset{\sim}{M}(\zeta):\zeta\varepsilon H\}$, then a real-valued function ϕ can be defined on M as

$$\phi[\underset{\sim}{M}(\zeta)] = \begin{cases} \Lambda_2'[\underset{\sim}{M}(\zeta)] & \text{if } \underset{\sim}{M}_{XX}(\zeta) \text{ is nonsingular} \\ -\infty & \text{otherwise.} \end{cases} \tag{30}$$

In this respect, the problem of finding a Λ_2'-optimal design for a multiresponse model is equivalent to finding a ϕ-optimal design for the single-response model (19) with $\underset{\sim}{h}'(\underset{\sim}{x}) = [\underset{\sim}{a}'(\underset{\sim}{x}): \underset{\sim}{b}'(\underset{\sim}{x})]$ as was seen earlier. The function ϕ defined in (30) can be shown to satisfy conditions (i), (ii), and (iii) described in Theorem 1. The proof of this theorem is given in Wijesinha and Khuri (1985).

Theorem 1. Let $M' = \{\underset{\sim}{M}(\zeta): \underset{\sim}{M}(\zeta)\varepsilon M$ and $\underset{\sim}{M}_{XX}(\zeta)$ is nonsingular$\}$. If $\Lambda_2'[\underset{\sim}{M}(\zeta)]$ is defined as in (29), then

(i) a Λ_2'-optimal measure exists.

(ii) Λ_2' is concave on M.

(iii) Λ_2' is differentiable on M'.

If $F_{\Lambda_2'}$ denotes the Fréchet derivative of Λ_2', then from Lemma 1 and Theorem 1 we may conclude that a design measure ζ^* is Λ_2'-optimal if and only if

$$\sup_{\underset{\sim}{x}\varepsilon X} F_{\Lambda_2'}\{\underset{\sim}{M}(\zeta^*),\ \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})\} = 0,$$

where $\underset{\sim}{h}'(\underset{\sim}{x}) = [\underset{\sim}{a}'(\underset{\sim}{x}): \underset{\sim}{b}'(\underset{\sim}{x})]$. This result will be used to construct a Λ_2'-optimal design in an iterative manner, just like in Silvey's (1980) procedure described in Section 4.1. First, we need to obtain an explicit expression for $F_{\Lambda_2'}$. This will be developed in the next theorem.

Theorem 2. If H is the set of all design measures on χ, then for $\zeta \varepsilon H$ and $\underset{\sim}{x} \varepsilon \chi$ we have

$$F_{\Lambda_2^{\prime}}\{\underset{\sim}{M}(\zeta),\ \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}^{\prime}(\underset{\sim}{x})\} = \mathrm{tr}[\underset{\sim}{T}^{-1}\underset{\sim}{L}\{\underset{\sim}{I}_r \otimes [\underset{\sim}{b}(\underset{\sim}{x}) - \underset{\sim}{v}(\underset{\sim}{x},\zeta)][\underset{\sim}{b}^{\prime}(\underset{\sim}{x}) - \underset{\sim}{v}^{\prime}(\underset{\sim}{x},\zeta)]\}\underset{\sim}{L}^{\prime}]$$
$$- \Lambda_2^{\prime}[\underset{\sim}{M}(\zeta)], \tag{31}$$

where $\underset{\sim}{v}(\underset{\sim}{x},\zeta) = \underset{\sim}{M}_{ZX}(\zeta)\underset{\sim}{M}_{XX}^{-1}(\zeta)\underset{\sim}{a}(\underset{\sim}{x})$ and $\underset{\sim}{h}(\underset{\sim}{x}) = [\underset{\sim}{a}^{\prime}(\underset{\sim}{x}):\underset{\sim}{b}^{\prime}(\underset{\sim}{x})]^{\prime}$.

Proof. For simplicity we shall write $\underset{\sim}{M}$ and $\underset{\sim}{h}$ instead of $\underset{\sim}{M}(\zeta)$ and $\underset{\sim}{h}(\underset{\sim}{x})$. By definition,

$$F_{\Lambda_2^{\prime}}(\underset{\sim}{M},\ \underset{\sim}{h}\underset{\sim}{h}^{\prime}) = \lim_{\varepsilon\to 0^+}(1/\varepsilon)\{\Lambda_2^{\prime}[\tilde{\underset{\sim}{M}}] - \Lambda_2^{\prime}[\underset{\sim}{M}]\},$$

where $\tilde{\underset{\sim}{M}} = (1-\varepsilon)\underset{\sim}{M} + \varepsilon\underset{\sim}{h}\underset{\sim}{h}^{\prime}$. Recall that

$$\Lambda_2^{\prime}[\underset{\sim}{M}] = \mathrm{tr}[\underset{\sim}{T}^{-1}\underset{\sim}{L}\{\underset{\sim}{I}_r \otimes (\underset{\sim}{M}_{ZZ} - \underset{\sim}{M}_{ZX}\underset{\sim}{M}_{XX}^{-1}\underset{\sim}{M}_{XZ})\}\underset{\sim}{L}^{\prime}].$$

Therefore,

$$F_{\Lambda_2^{\prime}}(\underset{\sim}{M},\ \underset{\sim}{h}\underset{\sim}{h}^{\prime}) = \lim_{\varepsilon\to 0^+}\mathrm{tr}\{\underset{\sim}{T}^{-1}\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{E})\underset{\sim}{L}^{\prime}\}, \tag{32}$$

where

$$\underset{\sim}{E} = (1/\varepsilon)\{\tilde{\underset{\sim}{M}}_{ZZ} - \tilde{\underset{\sim}{M}}_{ZX}\tilde{\underset{\sim}{M}}_{XX}^{-1}\tilde{\underset{\sim}{M}}_{XZ} - \underset{\sim}{M}_{ZZ} + \underset{\sim}{M}_{ZX}\underset{\sim}{M}_{XX}^{-1}\underset{\sim}{M}_{XZ}\}, \tag{33}$$

and

$$\tilde{\underset{\sim}{M}} = \begin{bmatrix} \tilde{\underset{\sim}{M}}_{XX} & \tilde{\underset{\sim}{M}}_{XZ} \\ \tilde{\underset{\sim}{M}}_{ZX} & \tilde{\underset{\sim}{M}}_{ZZ} \end{bmatrix} .$$

But from Dykstra (1971), for a nonsingular matrix $\underset{\sim}{A}$ we have the following identity:

$$(\underset{\sim}{A} + \underset{\sim}{x}_0\underset{\sim}{x}_0^{\prime})^{-1} = \underset{\sim}{A}^{-1} - \frac{\underset{\sim}{A}^{-1}\underset{\sim}{x}_0\underset{\sim}{x}_0^{\prime}\underset{\sim}{A}^{-1}}{1 + \underset{\sim}{x}_0^{\prime}\underset{\sim}{A}^{-1}\underset{\sim}{x}_0} .$$

Thus, if we let $\underset{\sim}{A} = (1-\varepsilon)\underset{\sim}{M}_{XX}$ and $\underset{\sim}{x}_0 = \varepsilon^{1/2}\underset{\sim}{a}$, we get

$$\tilde{\underset{\sim}{M}}_{XX}^{-1} = \{(1-\varepsilon)\underset{\sim}{M}_{XX} + \varepsilon\underset{\sim}{a}\underset{\sim}{a}^{\prime}\}^{-1}$$

$$= (1-\varepsilon)^{-1}\underset{\sim}{M}_{XX}^{-1} - \{\varepsilon c/(1-\varepsilon)^2\}\underset{\sim}{M}_{XX}^{-1}\ \underset{\sim}{a}\underset{\sim}{a}'\underset{\sim}{M}_{XX}^{-1},$$

where $c^{-1} = 1 + [\varepsilon/(1-\varepsilon)]\ \underset{\sim}{a}'\underset{\sim}{M}_{XX}^{-1}\ \underset{\sim}{a}$. It follows that

$\tilde{\underset{\sim}{M}}_{XX}^{-1} = (1-\varepsilon)^{-1}\underset{\sim}{M}_{XX}^{-1} - \{\varepsilon/t(1-\varepsilon)\}\underset{\sim}{P}$, where $t = 1 - \varepsilon + \varepsilon\underset{\sim}{a}'\underset{\sim}{M}_{XX}^{-1}\underset{\sim}{a}$ and $\underset{\sim}{P} = \underset{\sim}{M}_{XX}^{-1}\ \underset{\sim}{a}\underset{\sim}{a}'\underset{\sim}{M}_{XX}^{-1}$.

From (33) we obtain

$$\begin{aligned}\underset{\sim}{E} = {} & -\underset{\sim}{M}_{ZZ} + \underset{\sim}{M}_{ZX}\underset{\sim}{M}_{XX}^{-1}\underset{\sim}{M}_{XZ} + \underset{\sim}{b}\underset{\sim}{b}' - \underset{\sim}{M}_{ZX}\underset{\sim}{M}_{XX}^{-1}\ \underset{\sim}{a}\underset{\sim}{b}' - \underset{\sim}{b}\underset{\sim}{a}'\underset{\sim}{M}_{XX}^{-1}\underset{\sim}{M}_{XZ} \\ & - \{\varepsilon/(1-\varepsilon)\}\underset{\sim}{b}\underset{\sim}{a}'\underset{\sim}{M}_{XX}^{-1}\ \underset{\sim}{a}\underset{\sim}{b}' + \{(1-\varepsilon)/t\}\underset{\sim}{M}_{ZX}\underset{\sim}{P}\underset{\sim}{M}_{XZ} \\ & + (\varepsilon/t)\underset{\sim}{M}_{ZX}\underset{\sim}{P}\underset{\sim}{a}\underset{\sim}{b}' + (\varepsilon/t)\underset{\sim}{b}\underset{\sim}{a}'\underset{\sim}{P}\underset{\sim}{M}_{XZ} + \{\varepsilon^2/[(1-\varepsilon)t]\}\underset{\sim}{b}\underset{\sim}{a}'\underset{\sim}{P}\underset{\sim}{a}\underset{\sim}{b}'. \end{aligned} \tag{34}$$

From (32) and (34) we conclude that

$$\begin{aligned} & F_{\Lambda_2'}\{\underset{\sim}{M}(\zeta),\ \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})\} \\ & = \mathrm{tr}\ [\underset{\sim}{T}^{-1}\underset{\sim}{L}\{\underset{\sim}{I}_r \otimes [\underset{\sim}{b}(\underset{\sim}{x}) - \underset{\sim}{v}(\underset{\sim}{x},\zeta)][\underset{\sim}{b}'(\underset{\sim}{x}) - \underset{\sim}{v}'(\underset{\sim}{x},\zeta)]\}\underset{\sim}{L}'] - \Lambda_2'[\underset{\sim}{M}(\zeta)], \end{aligned}$$

where $\underset{\sim}{v}(\underset{\sim}{x},\zeta) = \underset{\sim}{M}_{ZX}(\zeta)\underset{\sim}{M}_{XX}^{-1}(\zeta)\underset{\sim}{a}(\underset{\sim}{x})$.

4.2 An Iterative Procedure to Obtain a Λ_2'-Optimal Design

Let $\underset{\sim}{h}(\underset{\sim}{x}) = [\underset{\sim}{a}'(\underset{\sim}{x}):\underset{\sim}{b}'(\underset{\sim}{x})]'$ and let $\underset{\sim}{M}(\zeta_N)$, $N > 1$, be defined as in (27). The main steps of the iterative procedure for constructing a Λ_2'-optimal design are:

1. Start with an initial design D_{N_0} (consisting of N_0 points) for which $\underset{\sim}{M}_{XX}(\zeta_{N_0})$ is nonsingular.

2. Obtain the design point $\underset{\sim}{x}_{N_0+1}$ at which $\sup_{\underset{\sim}{x}\in X} F_{\Lambda_2'}\{\underset{\sim}{M}(\zeta_{N_0}),\ \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})\}$ is attained.

3. Obtain D_{N_0+1} (hence ζ_{N_0+1}) by augmenting D_{N_0} with $\underset{\sim}{x}_{N_0+1}$. Recall that ζ_{N_0+1} is the design measure obtained by assigning probability $1/(N_0+1)$ to each design point in D_{N_0+1}.

4. Continue this process to find $\underset{\sim}{x}_{N_0+2}, \underset{\sim}{x}_{N_0+3}, \ldots,$ until

$$\sup_{\underset{\sim}{x} \in X} F_{\Lambda_2'}\{\underset{\sim}{M}(\zeta_N), \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})\} < \varepsilon, \tag{35}$$

for some $N > N_0$ and ε, where ε is a small positive number chosen a priori.

5. Numerical Examples

Example 1. One of the main concerns in industry is the determination of conditions on the controllable variables which lead to better yields and lower costs. In a paper by Lind et al. (1960), the authors discussed a case study of such a problem. They applied response surface techniques to a typical chemical processing operation. Three controllable variables were considered; they were x_1, x_2, and x_3 which represent, respectively, the proportions of two complexing agents, and the extraction pH level. The response variables were y_1 = percentage yield, y_2 = cost of materials (dollars per one kilogram of product). The controllable variables were coded so that $-1<x_i<1$ $(i=1,2,3)$. The fitted models are given below

$$E_a(y_i) = \beta_{i0} + \sum_{j=1}^{3} \beta_{ij} x_j + \beta_{i12} x_1 x_2 + \beta_{i13} x_1 x_3 + \beta_{i23} x_2 x_3, \quad i = 1,2.$$

If these models are inadequate, then it is necessary that the design be chosen so that the experimenter can quickly and efficiently detect the presence of lack of fit. In this case the design can be augmented with additional points to allow the fitting of models with higher-order terms. If, however, no significant lack of fit is detected, then the models can be used to determine conditions on x_1, x_2, and x_3 that lead to high yield-response values and low cost-response values. Let us consider that the true model for each response is of the second degree with all pure quadratic terms, i.e., x_1^2, x_2^2, and x_3^2 (this model was reported to be adequate according to the study by Lind et al., 1960).

The iterative procedure described in Section 4.2 was carried out using two initial designs given in Tables 1 and 2. The augmented design points, the $\sup_{\underset{\sim}{x} \in X} F_{\Lambda_2'}$ values, and the Λ_2' values are given in Tables 3 and 4. The figures indicate that the procedure has been successful in reducing the $F_{\Lambda_2'}$ values to a level very close to zero. A steady increase in the values of Λ_2' is also seen. It is quite clear from these results that the choice of the initial design has a significant effect on the location of the new design points as well as on the rate of convergence of the procedure.

Example 2. In this example we consider a multiresponse experiment with three responses, y_1, y_2, y_3, and three controllable variables, x_1, x_2, x_3, coded so that $-1 < x_i < 1$ $(i=1,2,3)$. The fitted models are

$$E_a(y_1) = \beta_{10} + \beta_{11}x_1 + \beta_{13}x_3 + \beta_{113}x_1x_3$$

$$E_a(y_2) = \beta_{20} + \sum_{j=1}^{3}\beta_{2j}x_j + \beta_{213}x_1x_3 + \beta_{211}x_1^2 + \beta_{233}x_3^2$$

$$E_a(y_3) = \beta_{30} + \sum_{j=1}^{3}\beta_{3j}x_j .$$

The true models are considered to be

$$E_t(y_1) = \beta_{10} + \beta_{11}x_1 + \beta_{13}x_3 + \beta_{113}x_1x_3 + \beta_{111}x_1^2 + \beta_{133}x_3^2$$

$$E_t(y_2) = \beta_{20}+\sum_{j=1}^{3}\beta_{2j}x_j+\beta_{213}x_1x_3+\beta_{211}x_1^2+\beta_{233}x_3^2+\beta_{212}x_1x_2+\beta_{223}x_2x_3+\beta_{222}x_2^2$$

$$E_t(y_3) = \beta_{30}+\sum_{j=1}^{3}\beta_{3j}x_j+\beta_{312}x_1x_2+\beta_{313}x_1x_3+\beta_{323}x_2x_3+\beta_{311}x_1^2+\beta_{322}x_2^2+\beta_{333}x_3^2$$

The initial design for this example is given in Table 5 and the augmented design points are given in Table 6. As in Example 1, we can clearly see that the proposed procedure has been effective in reducing the value of $\sup_{\underset{\sim}{x} \in X} F_{\Lambda_2'}[\underset{\sim}{M}(\zeta_{N-1}),\underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})]$ to a level arbitrarily close to zero.

Appendix

In this appendix we prove the inequality

$$\mathrm{tr}(\underset{\sim}{\Omega}) \geq e_{\min}(\underset{\sim}{\Sigma}^{-1})\underset{\sim}{\gamma}'\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{A})\underset{\sim}{L}'\underset{\sim}{\gamma}, \tag{A.1}$$

where

$\underset{\sim}{\gamma}' = [\underset{\sim}{\gamma}_1' : \underset{\sim}{\gamma}_2' : \cdots : \underset{\sim}{\gamma}_r']$, $\underset{\sim}{A} = \underset{\sim}{Z}_0' \{\underset{\sim}{I}_N - \underset{\sim}{X}_0(\underset{\sim}{X}_0'\underset{\sim}{X}_0)^{-1}\underset{\sim}{X}_0'\} \underset{\sim}{Z}_0$, and

$\underset{\sim}{L} = \mathrm{diag}(\underset{\sim}{H}_1', \underset{\sim}{H}_2', \ldots, \underset{\sim}{H}_r')$.

Proof

$$\mathrm{tr}[\underset{\sim}{\Gamma}'\underset{\sim}{Z}'\{\underset{\sim}{I}_N - \underset{\sim}{X}_0(\underset{\sim}{X}_0'\underset{\sim}{X}_0)^{-1}\underset{\sim}{X}_0'\}\underset{\sim}{Z}\underset{\sim}{\Gamma}]$$

$$= \sum_{i=1}^{r} \underset{\sim}{\gamma}_i'\underset{\sim}{H}_i'\underset{\sim}{A}\,\underset{\sim}{H}_i\underset{\sim}{\gamma}_i,$$

$$= [\underset{\sim}{\gamma}_1'\,\underset{\sim}{H}_1' : \underset{\sim}{\gamma}_2'\,\underset{\sim}{H}_2' : \cdots : \underset{\sim}{\gamma}_r'\,\underset{\sim}{H}_r'](\underset{\sim}{I}_r \otimes \underset{\sim}{A})[\underset{\sim}{\gamma}_1'\,\underset{\sim}{H}_1' : \underset{\sim}{\gamma}_2'\,\underset{\sim}{H}_2' : \cdots : \underset{\sim}{\gamma}_r'\,\underset{\sim}{H}_r']',$$

$$= \underset{\sim}{\gamma}'\,\underset{\sim}{L}(\underset{\sim}{I}_r \otimes \underset{\sim}{A})\,\underset{\sim}{L}'\underset{\sim}{\gamma}.$$

Inequality (A.1) follows from the above equality and inequality (7).

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Table 1. Initial Design 1 (Example 1).

x_1	x_2	x_3
1	1	1
1	1	-1
1	-1	1
1	-1	-1
-1	1	1
-1	1	-1
-1	-1	1
-1	-1	-1

Table 2. Initial Design 2 (Example 1).

x_1	x_2	x_3
-1.0	-0.5	-0.5
0.8	0.6	-0.7
0.4	-0.3	0.9
-0.2	0.8	1.0
0.5	-1.0	-1.0
-1.0	0.7	-1.0
-1.0	-1.0	1.0

Table 3. The Augmented Design Points using Initial Design 1 (Example 1).

N	$\underset{\sim}{x}_N$	$\sup_{\underset{\sim}{x} \in \mathcal{X}} F_{\Lambda_2^{*}} [\underset{\sim}{M}(\zeta_{N-1}), \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})]$	$\Lambda_2^{*} [\underset{\sim}{M}(\zeta_{N-1})]$
9	(-0.019,-0.008,-0.003)	67.4805	0.0000
10	(0.008,-0.001,-0.001)	4[illegible].6655	6.6644
11	(0.006, 0.006, 0.011)	32.4011	10.7976
12	(-0.002, 0.002,-0.009)	22.3158	13.3860
13	(0.007, 0.003, 0.016)	14.9971	14.9977
14	(-0.004, 0.011,-0.009)	9.5850	15.9737
15	(0.003, 0.012, 0.004)	5.5106	16.5279
16	(-0.001, 0.000,-0.005)	2.4048	16.7973
17	(0.000,-0.002, 0.000)	0.0050	16.8726

Table 4. The Augmented Design Points Using Initial Design 2 (Example 1).

N	$\underset{\sim}{x}_N$	$\sup_{\underset{\sim}{x} \in X} F_{\Lambda_2^-}[\underset{\sim}{M}(\zeta_{N-1}), \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})]$	$\Lambda_2^- [\underset{\sim}{M}(\zeta_{N-1})]$
8	(-1.000,-1.000,-1.000)	92.7738	0.0000
9	(0.880,-1.000, 0.280)	43.3311	2.1245
10	(-1.000, 0.891, 0.382)	40.6232	3.5374
11	(-0.241,-0.182,-0.089)	23.1349	4.7762
12	(0.902, 0.991, 0.881)	41.9346	6.6435
13	(-0.140,-0.079,-0.040)	17.9048	7.2794
14	(-0.139, 0.881,-1.000)	20.2792	8.4975
15	(-0.135,-0.060,-0.041)	12.8134	9.0801
16	(0.878,-0.223,-1.000)	14.6284	9.8342
17	(-0.120,-0.061,-0.059)	9.5272	10.1154
18	(-0.124,-0.063,-0.058)	6.7563	10.6228
19	(0.879, 0.900,-0.100)	11.9147	10.9438
20	(-0.161,-1.000,-0.079)	5.7707	11.1739
21	(-1.000,-0.019, 0.025)	5.0655	11.3401
22	(-0.120,-0.060,-1.000)	4.0475	11.4226
23	(0.920,-1.000, 0.890)	11.0403	11.5733
24	(0.883,-1.000,-1.000)	7.9772	11.5312
25	(0.043,-0.123,-0.043)	5.0573	11.5236
26	(0.045,-0.124,-0.045)	3.5450	11.6986
27	(-1.000, 0.891,-1.000)	7.0004	11.8117
28	(-1.000,-1.000, 0.880)	10.2624	11.8081
29	(-0.060,-0.120,-0.047)	4.1023	11.8672
30	(-0.100,-1.000,-0.040)	2.9559	11.9892
31	(-0.059,-0.119,-0.039)	2.4101	12.0441
32	(0.001,-0.009,-0.011)	1.0677	12.1065
33	(-0.003,-0.004,-0.000)	0.0156	12.1256

Table 5. The Initial Design for Example 2.

x_1	x_2	x_3
0.5	-0.6	0.3
1.0	1.0	-1.0
0.8	0.7	-1.0
1.0	0.3	-1.0
0.4	0.6	0.7
0.5	-0.8	0.9
1.0	-1.0	0.4

Table 6. The Augmented Design Points for Example 2.

N	$\underset{\sim}{x}_N$	$\sup_{\underset{\sim}{x} \in X} F_{\Lambda_2^-}[\underset{\sim}{M}(\zeta_{N-1}), \underset{\sim}{h}(\underset{\sim}{x})\underset{\sim}{h}'(\underset{\sim}{x})]$	$\Lambda_2^-[\underset{\sim}{M}(\zeta_{N-1})]$
8	(-1.000,-1.000,-1.000)	311006.8974	-0.0000
9	(-1.000, 0.880, 0.901)	496.1313	0.6116
10	(-1.000, 1.000,-1.000)	239.7514	0.8424
11	(0.620,-1.000,-1.000)	101.2637	4.0733
12	(-1.000,-1.000, 1.000)	132.6938	7.4027
13	(1.000, 0.995, 1.000)	118.0638	8.5210
14	(-1.000,-1.000,-0.120)	74.6300	8.3795
15	(1.000,-1.000,-1.000)	45.3371	10.4716
16	(-1.000, 0.880, 1.000)	24.9710	11.6581
17	(-1.000,-1.000, 0.995)	21.1408	12.0597
18	(-1.000, 0.880,-1.000)	10.7567	12.1594
19	(-1.000,-1.000,-1.000)	8.2219	12.1818
20	(1.000,-1.000, 0.894)	38.5043	12.1063
21	(1.000, 1.000, 1.000)	27.2943	12.7122
22	(1.000,-1.000,-1.000)	13.3531	13.1270
23	(-1.000, 0.880, 1.000)	10.5090	13.2994
24	(-0.940,-1.000, 0.899)	5.3225	13.4066
25	(1.000, 1.000,-1.000)	23.0393	13.3929
26	(-1.000, 0.898,-1.000)	7.5010	13.8408
27	(-1.000,-1.000,-1.000)	5.2012	13.8770
28	(1.000,-1.000,-1.000)	10.8382	13.8495
29	(1.000,-1.000, 1.000)	25.5676	14.0416
30	(1.000, 1.000, 1.000)	15.4512	14.2208
31	(-1.000, 0.894, 1.000)	7.0110	14.3827
32	(-1.000,-1.000, 0.880)	5.9191	14.4395
33	(-1.000,-1.000, 1.000)	1.5645	14.4925
34	(1.000, 1.000,-1.000)	16.9589	14.3978
35	(-1.000, 1.000,-1.000)	10.7206	14.6391
36	(-1.000,-1.000,-1.000)	4.4119	14.7352
37	(0.910,-1.000,-1.000)	3.8760	14.7178
38	(1.000,-1.000, 1.000)	16.9927	14.7342
39	(1.000, 1.000, 1.000)	11.9193	14.8585
40	(1.000, 1.000, 1.000)	1.8782	14.9712
41	(-1.000,-1.000,-1.000)	1.0772	14.9461
42	(1.000,-1.000,-1.000)	.01425	14.9103

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